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13. ABSTRACT (Maximum 200 words)

This research project consisted of a number of closely related topics involving researchers at several institutions. The research is leading to important new software tools and standards, using primarily, the software packages ScaLAPACK and P_ARPACK. ScaLAPACK, developed at the University of Tennessee at Knoxville, Oak Ridge National Laboratory, and the University of California at Berkeley, is a prototype library of software for performing dense and band linear algebra computations on message-passing computers. P_ARPACK, developed at Rice University, is a distributed-memory software package for solving large, sparse, nonsymmetrical eigenproblems using a variant of the implicitly restarted arnoldi method.

Recognizing that a message passing standard was necessary to ensure the easy portability of the prototype libraries, the project initiated and promoted the development of the MPI message passing interface, as well as the HPF standard. Standards specific to parallel linear algebra are also being developed.

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A Scalable Parallel Library for Numerical Linear Algebra

Final Progress Report
Jack J. Dongarra
July 1999

U.S. Army Research Office

Research Agreement DAAH04-95-1-0077

University of Tennessee at Knoxville
Oak Ridge National Laboratory
University of California at Berkeley
Rice University
University of Illinois at Urbana-Champaign
University of California at Los Angeles

Contents

1 Problem Studied

This report surveys final progress in the research project "A Scalable Parallel Library For Numerical Linear Algebra," and constitutes a final progress report.

This research project consisted of a number of closely related topics involving researchers at a number of institutions. ScaLAPACK is being developed at the University of Tennessee at Knoxville, Oak Ridge National Laboratory, and the University of California at Berkeley. ScaLAPACK is a prototype library of software for performing dense and band linear algebra computations on message-passing computers, and also includes out-of-core linear solvers, out-of-core eigensolvers, new ScaLAPACK and PBLAS routines for packed storage, an HPF interface to a subset of ScaLAPACK routines, SuperLU, SuperLU_MT, and SuperLU_DIST, a spectral divide and conquer (SDC) eigensolver using the matrix sign function, and ATLAS.

P_ARPACK is developed at Rice University, and is a distributed-memory software package for solving large, sparse, nonsymmetric eigenproblems using a variant of the implicitly restarted Arnoldi method. CAPSS, developed at the University of Illinois at Urbana-Champaign, is a fully parallel package for solving sparse linear systems of the form $Ax = b$ on message passing computers using matrix factorization. Researchers at the University of Tennessee at Knoxville and the University of California at Los Angeles are developing a package called ParPre which is a collection of parallel preconditioners for iterative solution methods for linear systems of equations. ScaLAPACK, P_ARPACK, CAPSS, and ParPre have been placed in the public domain and are accessible via the National HPCC Software Exchange.

`http://www.netlib.org/scalapack/`

The research is leading to a number of important new software tools and standards. Recognizing that a message passing standard was necessary to ensure the easy portability of the prototype libraries, the project initiated and promoted the development of the MPI message passing interface [4], as well as the HPF [5] standard. Standards specific to parallel linear algebra are also being developed.

2 Summary of Most Important Results

The official release of the PBLAS, version 2.0, was announced in FY 1999. This new release of the PBLAS will be included in the next release of ScaLAPACK, projected for the year 2000. Also included in the next release of ScaLAPACK will be the parallel divide and conquer symmetric eigensolver that was developed in FY 1998.

SuperLU is a supernodal version of sparse Gaussian elimination and is currently one of the two fastest serial implementations of sparse Gaussian elimination (on some test problems it wins, on others another code is faster), and the fastest parallel implementation. Serial SuperLU, multi-threaded SuperLU_MT, and distributed-memory SuperLU_DIST are available on netlib.

We have a prototype running of a new algorithm, which may be the ultimate solution for the symmetric eigenproblem on both parallel and serial machines. This algorithm has been incorporated into the symmetric eigenproblems of LAPACK, version 3.0, and will soon be propogated into the SVD, and the SVD-based least squares solver. We expect to also propagate this algorithm into ScaLAPACK.

ARPACK++: A C++ interface has been developed for ARPACK. This package provides templates for utilizing ARPACK in an object oriented environment. All of the Fortran templates provided in the EXAMPLES directory are available in a high level form that requires little more than a matrix definition and specification of which eigenvalues to compute from the user. Shift-Invert spectral transformation modes incorporate and use the SuperLU sparse factorization software mentioned previously in this report. This software is complete and is undergoing Beta-test now. Further testing and refinement should be completed within the next six months. This will then be made a part of the regular ARPACK distribution on completion.

We have continued developing a blocked out-of-core variant of the implicitly restarted Arnoldi method, as well as improved spectral transformation strategies and deflation techniques for large sparse eigenvalue problems.

Our work has been adopted by Mathworks and forms the basis for the new *eigs* command in Matlab for sparse eigenvalue computation.

We have completed an ARPACK users guide that is currently available on the web:

R.B. Lehoucq, D.C. Sorensen, and C. Yang,
ARPACK Users Guide: Solution of Large Scale Eigenvalue Problems with Implicitly Restarted Arnoldi methods, 142 pages, SIAM Publications (1998)

A user's guide for ARPACK++ has been completed and is currently available from `http://www.caam.rice.edu/software/ARPACK`.

F.M. Gomes and D.C. Sorensen,
ARPACK++ : A C++ implementation of the ARPACK eigenvalue package (draft date June 1997).

The main effort for the CAPSS project was directed towards developing a scalable "Domain-separator ICCG" by for large-scale multiprocessors. This is a major development and integration effort and involves adapting several components of CAPSS and MFACT as well as implementing new algorithms. For example, we will replace numeric kernels for multifrontal factorization (in CAPSS) by a new tree-update scheme with flexible matrix forms. Likewise, for applying the preconditioner we will modify SI to work with our new, flexible matrix forms. Furthermore, we will add a post-processing step to drop small elements.

The plans for our object-oriented framework for grid solvers focused on completing the design and implementation of the factorization phases as part of the object-oriented framework, to be followed by the design and implementation of the grid-based preconditioner for iterative methods, and then demonstrating the capabilities of the object-oriented framework on various grid-based applications.

Plans for the interactive framework DLab call for expanding its repertoire of operations to include support for sparse matrix computations and fast Fourier transforms. Substantial refinements are planned for DLab's scheduler, resource monitor, and its performance prediction and lazy evaluation capabilities. This work was presented in a minisymposium at the SIAM National Meeting in Atlanta in May, 1999.

The ParPre library now comprises Schwarz preconditioners, Schur-complement domain decomposition methods, block SSOR/ILU preconditioners, and V-cycle multilevel methods. The multilevel methods are both parallel multi-colour ILU, and algebraic multigrid type methods. The code is being maintained to keep it compatible with the Petsc library, and we are doing further research into the multilevel methods. Web site for the ParPre project:

```
http://www.cs.utk.edu/~eijkhout/parpre.html
```

A manual for ParPre as well as a paper on the design principles have been published [3, 2].

We have rewritten some of the internals of ParPre to reflect changes in the design of the PETSc library, which we use. The functionality of the Block SSOR method has been expanded so that it can reproduce various block factorizations, including an exact factorization.

We have identified several aspects of the algebraic multilevel method in which the parallel method is fundamentally different from earlier sequential ones. We are investigating these, and update the code to reflect the new insights.

We have begun research into the existence question of incomplete factorizations. Such sequential methods are crucial as local components of various types of domain decomposition methods.

We will continue the further development of algebraic multilevel methods and perform extensive testing on them. In addition, we intend to supply a proof of the condition number reduction of the method, analogous to such proofs as in [1].

ATLAS was extended in FY 1998 to support the matrix-vector multiply DGEMV, and will eventually generate all Level 3 BLAS directly, as well as providing complex data types. Much of the technology and approach developed here can be applied to the other Level 3 BLAS and the general strategy can have an impact on basic linear algebra operations in general and may be extended to other important kernel operations.

Another avenue of research for ATLAS involves sparse algorithms. The fundamental building block of iterative methods is the sparse matrix times dense vector multiply. This work should leverage the present research (in particular, make use of the dense matrix-vector multiply). The present work uses compile-time adaptation of software. Since matrix vector multiply may be called literally thousands of times during the course of an iterative method, we plan to investigate run-time adaptation as well. These run-time adaptations could include matrix dependent transformations [6], as well as specific code generation. For further details, please refer to the following URL:

```
http://www.netlib.org/atlas/
```

The BLAS Technical Forum meetings continued through 1998. On

April 27-29, 1998, the meeting was held at SGI/Cray Research in Eagan, Minnesota. The next meeting was held at NIST in Washington, D.C. on October 8-9, 1998. And on December 14-16, 1998, the meeting was held at LBL in Berkeley, California. The final meeting occurred on March 16-18, 1999, at the Ramada Inn and Suites in Oak Ridge, TN.

Refer to the BLAS Technical Forum homepage

`http://www.netlib.org/utk/papers/blast-forum.html`

for detailed minutes from each of the meetings and a draft of the document for the BLAS Standard. Reference implementations of the proposed routines are being written. The final draft of the BLAS Standard will be available in the Summer, 2000.

And finally, a large team of experts is working on a book of Eigentemplates, which is designed to help the user find the best eigenvalue algorithm available for a particular problem and computer. The book is entering the final stage of the editing, and we are expecting to have the eigentemplate book published by SIAM in the Fall, 1999. The current draft of the book is available via the URL:

`http://www.ms.uky.edu/~bai/ET/contents.html`

Technology Transfer

The ScaLAPACK library for dense linear algebra computations is in the process of transition to the commercial marketplace. ScaLAPACK has been incorporated into several commercial packages, including the NAG Parallel Library, IBM Parallel ESSL, and SGI Cray Scientific Software Library, and is being integrated into the VNI IMSL Numerical Library, as well as software libraries for Fujitsu, Hewlett-Packard/Convex, Hitachi, and NEC.

The ScaLAPACK library has become an official release for ASCI Red's operating system. Each build of the operating system will be validated against ScaLAPACK and each new compiler and operating system drop will contain an automatically generated fresh ScaLAPACK build. It will be in /usr/lib, as standard as the BLAS.

The ScaLAPACK generalized Hermitian eigensolver is being enhanced and has being incorporated into the electron structure MP-Quest project at Sandia National Laboratory. It is approximately ten

times faster than the previously existing eigensolver in MP-Quest, and will result in an approximate 90an entry for the Gordon Bell competition based on this work. Performance enhancements to the eigencode will be propagated into the next ScaLAPACK release.

The point of contact for ScaLAPACK is Susan Blackford, (865) 974-5886, susan@cs.utk.edu.

The ARPACK work has been adopted by Mathworks and forms the basis for the new *eigs* command in Matlab for sparse eigenvalue computation. We have entered into a collaboration with Roldan Pozo of NIST to construct an interface between ARPACK++ and TNT. This will provide the ability to define and work with matrices in ARPACK++ using TNT matrix classes. We have also established a research relationship with Sandia Albuquerque. Parallel ARPACK has been linked to AZTEC (Sandia's parallel iterative linear solver package) and is being applied to a stability analysis of thin film reactors. The point of contact for ARPACK, ARPACK++, and P_ARPACK is Dr. Dan Sorensen, (713) 527-4805, sorensen@rice.edu.

CAPSS has been used in solving numerous problems in structural mechanics, including shearing in foam-like materials and crack propagation in extrusion processes. CAPSS has also been used in the study of fluid-flows using higher-order finite-element methods. MFACT and CAPSS are being used to solve large-scale complex systems from electromagnetic applications at Northop-Grummann. The point of contact for CAPSS is Dr. Mike Heath, (217) 333-6268, heath@ncsa.uiuc.edu.

3 Publications and Technical Reports

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17. *Implementation in ScaLAPACK of Divide and Conquer Algorithms for Banded and Tridiagonal Linear Systems*, A. Cleary and J. Dongarra, University of Tennessee Technical Report, CS-97-358, 1997 (also LAPACK Working Note 125).

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59. *Convergence Analysis of an Inexact Truncated RQ-Iteration*, C. Yang, Rice University CAAM-TR98-07, 1998. (Submitted to Electronic Transactions on Numerical Analysis).

4 Participating Scientific Personnel Earning Advanced Degrees

- Inderjit Dhillon, Graduate Student, University of California at Berkeley, PhD 1997.
- Jennifer Finger, Graduate Student, University of Tennessee at Knoxville, MS 1997.
- Thomas Harrold, Graduate student, University of Tennessee at Knoxville, MS 1997.
- Jeff Horner, Graduate student, University of Tennessee at Knoxville, MS 1999.
- Song Jin, Graduate Student, University of Tennessee at Knoxville, MS 1999.
- Youngbae Kim, Graduate student, University of Tennessee at Knoxville, PhD 1996.
- A. Oliveira, Graduate student, Rice University, PhD 1997.
- Antoine Petitet, Graduate student, University of Tennessee at Knoxville, PhD 1996.
- Huan Ren, Graduate Student, University of California at Berkeley, PhD 1997.
- Howard Robinson, Graduate Student, University of California at Berkeley, MS 1997.
- M. Rojas, Graduate student, Rice University, PhD 1998.
- Ken Stanley, Graduate student, University of California at Berkeley, PhD 1997.
- C. Yang, Graduate student, Rice University, PhD 1998.

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